

Thiodiphosphoric acid ($[(\text{HO})_2\text{P}(\text{S})]_2\text{O}$), tetraethyl ester

Other names:

ASP 47
Bay-E-393
Bayer-E 393
Bis(O,O-diethylphosphorothionic) anhydride
Bladafum
Bladafume
Bladafun
Di(thiophosphoric) acid, tetraethyl ester
Dithiodiphosphoric acid, tetraethyl ester
Dithiofos
Dithion
Dithione
Dithiophos
Dithiopyrophosphate de tetraethyle
Dithiopyrophosphoric acid, tetraethyl ester
Dithiotep
E393
ENT 16,273
Ethyl thiopyrophosphate
Ethyl thiopyrophosphate ($[(\text{EtO})_2\text{PS}]_2\text{O}$)
Fulex
Lethalaire G-57
NSC 66403
O,O,O'-Tetraethyl dithiopyrophosphate
O,O,O,O-Tetraethyl-dithionopyrophosphat
O,O,O,O-Tetraethyl Dithiopyrophosphate
O,O,O,O-Tetraethyl-dithio-difosfaat
O,O,O,O-Tetraetil-ditio-pirofosfato
Pirofos
Plant dithio aerosol
Plantfume 103 smoke generator
Pyrophosphoric acid, tetraethyldithio-
Pyrophosphorodithioic acid, O,O,O,O-tetraethyl ester
Pyrophosphorodithioic acid, tetraethyl ester
Rcra waste number P109
Sulfatep
Sulfotep
Sulfotepp
TEDP
TEDTP

Tetraethyl dithionopyrophosphate
Tetraethyl dithiopyrophosphate
Tetraethyldithiodifosfat
Thiodiphosphoric acid tetraethyl ester
Thiopyrophosphoric acid ([$(\text{HO})_2\text{PS}]_2\text{O}$), tetraethyl ester
Thiopyrophosphoric acid, tetraethyl ester
Thiotepp
UN 1704

Inchi: InChI=1S/C8H20O5P2S2/c1-5-9-14(16,10-6-2)13-15(17,11-7-3)12-8-4/h5-8H2,1-4H3
InchiKey: XIUROWKZWPIAIB-UHFFFAOYSA-N
Formula: C8H20O5P2S2
SMILES: CCOP(=S)(OCC)OP(=S)(OCC)OCC
Mol. weight [g/mol]: 322.32
CAS: 3689-24-5

Physical Properties

Property code	Value	Unit	Source
hvap	77.86	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-4.40		Cheméo Relay (1.0)
logp	3.598		Crippen Method
mcvol	226.550	ml/mol	McGowan Method
rinpol	1675.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	582.75	K	Cheméo Relay (1.0)
tf	212.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	80.60	kJ/mol	351.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.23753e+01
Coeff. B	-9.69780e+03
Temperature range (K), min.	439.06
Temperature range (K), max.	568.33

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3689245&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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